Electron space charge effect on spin injection into semiconductors

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We consider spin polarized transport in a ferromagnet-insulator/semiconductor/insulator-ferromagnet (F1-I-S-I-F2) junction. We find that the spin current is strongly dependent on the spin configurations, the doping and space charge distribution in the semiconductor. When the ferromagnet-semiconductor interface resistance is comparable to the semiconductor resistance, the magnetoresistance ratio of this junction can be greatly enhanced under appropriate doping when the space charge effect in the nonequilibrium transport processes is taken into consideration.

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There is much interest recently in incorporating magnetic elements into semiconductor structures. One of the current focus lies in injecting spin polarized electrons into non-magnetic semiconductors [1–7]. This is partially motivated by the high magnetoresistance observed in ferromagnet tunnel junctions [8]. However, experiments have so far observed a small magnetoresistance ratio of 1% [9,10] in F-S-F structures. Schmidt et al [11] emphasized that the large resistance of the nonmagnetic semiconductor dominates the total resistance and thus lowers the magnetoresistance ratio. A similar discussion based on a ballistic picture was given by Grundler [12] and Hu et al [7]. Rashba pointed out that in a ferromagnetic metal/insulator/semiconductor (FIS) junction the resistance of the barrier insulator layer can be comparable to that of the semiconductor, $\Delta R/R$ may be raised by a considerable percentage [13]. Many different geometries of the tunneling junction were discussed in Ref. [14].

Although it is possible that to lift the magnetoresistance to near 10% with a very high electric field [15], there is no a low field scenario yet. On the other hand, the effect of the Coulomb interaction between the electrons in the non-magnetic semiconductor in the nonequilibrium transport process was not taken into consideration in the above mentioned works. In previous works on the ferromagnetic metal/insulator/ferromagnetic metal junction [16], one of us found that this interaction between the electrons in nonequilibrium transport processes played an important role in the characteristics of the device. Under steady state nonequilibrium conditions, a magnetization dipole layer much larger than the charge dipole layer is induced at the interface. The magnetization dipole layer is zero under equilibrium conditions. In this paper, we consider the role played by the Coulomb interaction in an F1-I1-S-I2-F2 junction. To completely solve the nonequilibrium transport processes with interactions is highly non-trivial. It requires solving self consistently Boltzmann type spin transport equation with the Poisson equation. What we want to touch in this work is using a simple Hartree approximation to check if the effect comes from the interactions is significant. We found that the spin polarized current is strongly affected by the interaction in this approximation. Because of the large difference in the spin-dependent current between the parallel and anti-parallel configurations, which is caused by the space charge effect, the total resistance becomes dependent on the spin configuration. We found that magnetoresistance ratio $\Delta R/R$ can be increased by one order of magnitude higher than the result obtained without the interactions under appropriate doping of the semiconductor. Typically, $\Delta R/R \sim 3\%$ for the non-interaction electrons while $\Delta R/R$ may attain values as high as $\sim 50\%$ due to the space charge. (See, Figures 2 and 3 below.) We also study another physical observable, the polarization $P = \frac{j_+ - j_-}{j_+ + j_-}$ and find that it is strongly dependent on the space charge distribution. We now describe our result in detail.

General description: We consider the junction F1-I1-S-I2-F2. The thickness of the metal (F1, F2), the insulating barriers (I1, I2) and the semiconductor (S) are denoted by $L^{L,R}$, $d_{1,2}$ and x_0 , respectively (See, Figure 1). For the practical case, x_0 is less than the spin diffusion length in the semiconductor l_N . The charge screening lengths in the metal and the semiconductor are denoted by $\lambda_{L,R}$ and λ_N , respectively. In our model, we assume $\lambda_N \ll$ l_N and $\lambda_{R,L} \ll l_{R,L}$, the spin diffusion lengths in the metal. Typically, $\lambda \sim 10^{-1} \text{nm}$, $l \sim 10^{1} \text{nm}$, and $l_N >$ $1\mu \text{m}$. $x_0 \sim 100 \text{nm}$ to $1\mu \text{m}$, depending on the structure of junctions. The screening length in the semiconductor, λ_N , is dependent on the doping of the semiconductor and can vary in a wide range, say 10nm for the heavy doped semiconductor and $100\text{nm}-1\mu\text{m}$ for the lightly doped or undoped semiconductor.

The problem we would like to solve is defined by the following four sets of equations.

(1) The first is the total charge-current conservation,

$$\nabla \cdot \mathbf{j} = -\frac{\partial \rho}{\partial t},\tag{1}$$

where ρ is the charge density.

(2) The second is the diffusion equations of the spin s-dependent current. In order to allow an analytic analysis, we take a simple Hartree approximation into account to see the space charge effect. Under such an approximation, the diffusion equations reads [16]

$$j_s = \sigma_s(\nabla \mu_s - \nabla W_0 + E),\tag{2}$$

where the magnitude of the electric charge has been set as one; E is the external electric field; the chemical potential μ_s is related to the charge density ρ_s by $\nabla \mu_s = \frac{\nabla \rho_s}{N_s}$ where N_s is the spin-dependent density of state. $W_0 = \int d\vec{r}' U_{int}(\vec{r} - \vec{r}') \rho(\vec{r}')$ is the potential caused by the screened Coulomb interaction $U_{int}(\vec{r})$ and ∇W_0 is the so-called screening field induced by $U_{int}(\vec{r})$. (In the present device geometry, the three dimensional integration is reduced to a one-dimensional one.)

(3) The third is the magnetization relaxation equation where the magnetization density $M = \rho_{\uparrow} - \rho_{\downarrow}$ relaxes with a renormalized spin diffusion length l. In the relaxation time approximation, one has

$$\nabla^2 M - M/l^2 = 0. (3)$$

(4) The fourth is the boundary condition at the interfaces

$$\Delta \tilde{\mu}_s - \Delta W = r(1 - s\gamma)j_s,\tag{4}$$

where $\tilde{\mu}_s = \mu_s + Ex$; Ex is the voltage drop on the left side of the barrier and ΔW is the electric potential drop across the barrier, which is assumed much smaller than $\Delta \mu_s$; $r_s = r(1-s\gamma)$ is the barrier resistance. We assume that there is no spin relaxation in the insulator, the spin-dependent currents are continuous across the junctions, $j_s^L(-d_1/2) = j_s^N(d_1/2)$ and $j_s^R(x_0 + d_2/2) = j_s^N(x_0 - d_2/2)$.

In addition, we have the neutrality condition for the total charges $(Q_{L,N,R}, \text{ e.g.}, Q_N = \int_{d_1/2}^{x_0+d_1/2} \rho dx)$ accumulated at the interfaces. By Gauss' law, for the point $d_1/2 < x < x_0 + d_1/2$, i.e., inside the semiconductor, the potential W_0 is determined by

$$\nabla W_0(x) = 4\pi Q_L + 4\pi \int_{d_1/2}^x \rho dx,$$
 (5)

whose constant part of the right hand side gives the constraint on the charge while the x-dependent part gives the function form of the potential W_0 . Another constraint is the neutrality of the system:

$$Q_L + Q_N + Q_R = 0. (6)$$

With those sets of equations (Eqs.(1)-(4)) and the two constraint on the charges (Eqs.(5) and (6)), the problem can be solved. The formal solutions of the problem are

$$\rho^{L}(x) = \frac{\lambda_{L}}{l_{L}} \rho_{10}^{L} e^{(x+d_{1}/2)/\lambda_{L}} + \frac{\lambda_{L}^{2}}{l_{L}^{2}} \rho_{20}^{L} e^{(x+d_{1}/2)/l_{L}},$$

$$M^{L}(x) = M_{0}^{L} (1 - \frac{\lambda_{L}^{2}}{l_{I}^{2}}) e^{(x+d_{1}/2)/l_{L}},$$
(7)

with similar solutions for the right hand side. In the semiconductor, if $\lambda_N \ll x_0$,

$$\rho^{N}(x) = \rho^{(1)}(x) + \rho^{(2)}(x),$$

$$\rho^{(1)}(x) = \frac{\lambda_{N}}{l_{N}} \rho_{10}^{(1)} e^{-(x-d_{1}/2)/\lambda_{N}} + \frac{\lambda_{N}^{2}}{l_{N}^{2}} \rho_{20}^{(1)} e^{-(x-d_{1}/2)/l_{N}},$$

$$\rho^{(2)}(x) = \frac{\lambda_{N}}{l_{N}} \rho_{10}^{(2)} e^{(x-x_{0}+d_{2}/2)/\lambda_{N}} + \frac{\lambda_{N}^{2}}{l_{2}^{2}} \rho_{20}^{(2)} e^{(x-x_{0}+d_{2}/2)/l_{N}}.$$
(8)

 $M^{(1),(2)}$ can be obtained similarly. All of coefficients in (7) and (8) can be determined by using Eqs.(1)-(4) and the constraint (5) and (6). The screening potential W_0 is determined by Gauss' law. The total current is $j = \sum_s j_s$. Although j_s are not a constant, the total current j is still a constant.

The spin-dependent current: To demonstrate the essential physics, we simplify matters by setting the parameters of the metals and barrier widths on the left and right sides to be the same: $\lambda_R = \lambda_L = \lambda$, $l_L = l_R = l$, $d_1 = d_2 = d$ and so on. The resistances of the barrier layers are taken as $r^{(1)} = r^{(2)} = r$; $\gamma_1 = \gamma_2 = \gamma$ for the parallel configuration and $\gamma_1 = -\gamma_2 = \gamma$ for the anti-parallel configuration. To illustrate, we focus on the calculation in the left barrier located at x = 0. The tunneling resistance is given by $r_s^{(1)} = r(1 - \gamma s) = r_{0,s} \exp[d(\kappa_s(\mu) - \kappa_s(0))]$, where $\kappa_s(\mu) \propto \int_0^d dx [2m(U - \Delta \mu_s(0)x/d)]^{1/2}$, with U the barrier height. That is $\kappa_s(\mu) = \kappa_{0,s} \frac{2}{3\Delta \hat{\mu}_s(0)} [1 - (1 - \Delta \hat{\mu}_s(0))]^{3/2}$. Here $\Delta \hat{\mu}_s = \Delta \mu_s/U$. The current $j_s^L(x)$ at x = 0 is dependent on the bias voltage and the space charge distribution, which is given by

$$j_s^L(0) = A_s j_{0s}, (9)$$

where

$$A_s = 1 + \frac{4\pi\lambda^2}{l} \frac{\alpha(\beta - s)}{1 - \alpha\beta} \frac{\rho_{10}^L + M_0^L}{E},\tag{10}$$

and $j_{0s} = \sigma_s E$ is the current with no interaction; β (α) measures the spin asymmetry of the conductivities σ_s (densities of states at the Fermi surface N_s): $\sigma_s = \frac{\sigma}{2}(1 + \beta s)$ and $N_s = \frac{1}{2}N_F(1 + s\alpha)$ where N_F is related to the screening length λ by $\frac{1}{N_F} = 2\pi\lambda^2\frac{1-\alpha^2}{1-\alpha\beta}$. Noting that both ρ_{10}^L and M_0^L are proportional to the external electric field E, A_s is solely determined by the material parameters.

Eq. (9) implies that the spin-dependent current $j_s(0)$ passing the interface differs a factor A_s from the non-interacting current $j_{0s}(0)$ which, for the parallel configuration, is given by

$$j_{0s}^{s}(0) \approx \frac{V}{R_N + 2r_{0.s}Y_s(0)},$$
 (11)

where $Y_s(0) = e^{\kappa_{0s}d[\frac{2}{3\Delta\hat{\mu}_s(0)}(1-(1-\Delta\hat{\mu}_s(0))^{3/2})-1]}$. For the anti-parallel configuration,

$$j_{0s}^{a}(0) \approx \frac{V}{R_N + \sum_{s} r_{0.s} Y_s(0)},$$
 (12)

which is almost spin-independent.

The magnetoresistance: Since the total current is constant everywhere, we have, for the parallel configuration

$$\frac{1}{R_P} = \sum_s j_s(0)/V = \sum_s \frac{A_s^P}{R_N + 2r_{0,s}Y_s^P(0)},$$
 (13)

and for the anti-parallel configuration, we have

$$\frac{1}{R_{AP}} = \sum_{s} j_s(0)/V = \frac{2}{R_N + \sum_{s} r_{0,s} Y_s^{AP}(0)}.$$
 (14)

From these, we obtain the magnetoresistance ratio

$$\frac{\Delta R}{R} \equiv \frac{R_{AP} - R_P}{(R_{AP} + R_P)/2} = \frac{2X}{2 + X},$$

$$X = \sum_{s} \frac{A_s^P (R_N + \sum_{s'} r_{0,s'} Y_{s'}^{AP}(0))}{2(R_N + 2r_{0,s} Y_s^P(0))} - 1.$$
(15)

For non-interacting electrons, $A_{+}^{P} = A_{-}^{P} = 1$ and one can see that $\Delta R/R$ will not be beyond a maximal value (at $V \to 0$) about 3.23% for $r_{0+} : r_{0-} : R_N = 1 : 2 : 1$ and decays as the bias voltage increases. In Fig. 2, we plot the bias-dependence of the magnetoresistance ratio for both the non-interacting and the interacting case with $x_0 \sim 1.25 \mu \text{m}$. Here we take $\lambda = 0.1 \text{nm}$, l = 20 nm, $\alpha = \beta = 1/2$ and $l_N = 3\mu \text{m}$ [17]. After the space charge effect is included, the ratio (15) grows as λ_N becomes smaller. This screening length can be controlled by doping the semiconductor (or by applying an external gate voltage). The small λ_N requires heavy doping of the semiconductor. For a heavily doped semiconductor, it may arrive at the giant magnetoresistance value, say 56% as shown in the figure, which raises orders of the magnitude comparing to the magnetoresistance for the non-interacting electrons.

There are some points to be emphasized in our calculations. i) In the large R_N limit, $\Delta R/R$ tends to zero no matter if there is any interaction effect. ii) At zero bias, the magnetoresistance is highest. In Fig. 2, we show the dependence of the magnetoresistance ratio on λ_N/x_0 for different $x_0(\gg l)$ at zero bias [18]. For a given x_0 , we see the magnetoresistance is also dependent on l. iii) The magnetoresistance is reduced as the bias voltage increases. We expect that the effective barrier height U, say several voltage, for the FIS interface to be larger than that for the F-I-F structure because the work function of the semiconductor is smaller than that of a metal. So on an absolute scale of voltage, this effect is not as big as in the conventional F-I-F structure. Namely, the large magnetoresistance can be anticipated at an experimental relevant bias voltage.

The polarization: We consider another experimental measurable quantity [5], the polarization of current, which is defined by $P = \frac{j_+(0)-j_-(0)}{j_+(0)+j_-(0)}$. We first calculate P by ignoring the space charge effect. In the antiparallel configuration P is nearly zero. The polarization P for the parallel configuration is also small if R_N

dominates but it may arrive a considerable magnitude if the r_{0s} is of the same order of R_N , e.g., if the ratio $r_{0+}:r_{0-}:R_N=1:2:1$, it may arrive at 40% at the zero bias. (In a wide range, our result is not very sensitive to this ratio if these resistances have the same order of magnitude.) P decays as the bias voltage increases, say for $V/U \sim 1$, P drops to less than 10%.

To see the space charge effect, we look at A_s . We found that A_s are nearly independent of l_N if l_N is the longest length scale. We fix $l_N = 3\mu \text{m}$ and $\kappa_{0s}d = 300$. For the anti-parallel configuration, the polarization is given by $P^{ap} = \frac{A_+ - A_-}{A_+ + A_-}$, which is bias-independent. In a large screening length λ_N and x_0 , e.g., 100nm and 1.5 μ m, P^{ap} is of the same order of the magnitude as that in the noninteracting case. However, for a small λ_N and x_0 , e.g., 30 nm and $0.5\mu m$, P^{ap} can be larger than one because j_+ , j_{-} can go in opposite directions. P^{ap} becomes significant when λ_N and x_0 are getting smaller. The physics behind this phenomenon can not be well-understood yet at this stage. An intuitive consideration is as follows: The effective driving potential $\Delta \mu_s$ is different in sign between spin up and spin down electrons, because the net charge density at the interface is less than the magnetization density [16]. This inequality can be traced to stem from the fact that the magnetic length is much larger than the screening length. Because of this sign difference of the driving potential, the currents for the two spin components may go in opposite directions. However, this consideration has to be examined thoroughly and we shall leave it to the further works. The polarization of the parallel configuration is bias dependent. For a large λ_N and small x_0 (say 100 nm and 0.5μ m), P^p decays as the bias voltage increases. However, for a small λ_N (say 30 nm) and large x_0 (say $2\mu m$), P^p increases as the bias voltage and finally saturates. However, these bias dependent effects happen only in the high bias regime, say V/U > 1. Thus, for the practical usage, this bias dependence may not be so important.

In conclusions, we have considered the space charge effect in a multiple FIS junction. In the Hartree approximation, we found a conspicuous difference of the spindependent current in the parallel configuration from that in the non-interaction models while the difference is minor for the anti-parallel configuration. This leads to an order of magnitude growing in the magnetoresistance ratio in such an approximation from the non-interaction model if the parameters of the junction are appropriately chosen. Although our theory is based on a specific junction geometry and a simple approximation, it has indicated that the electron interaction may play an important role in nonequilibrium transport processes for some types of spintronic devices on the spin injection. To quantitatively solve the nonoequilibrium transport processes, a stricter treatment is required.

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- [17] Throughout this paper, we take this set of the parameters in all numerical results. For other values of α and β , there will not be a qualitative change if they are not very close to 0 or 1.
- [18] In the regime where x_0 and λ_N are of the order of l, the situation is a bit subtle and requires more researches. Our investigation is limited in $\lambda_N \ll x_0$.

Fig. 1 The sketch of the geometry of the junction. The quantities of the left (right) ferromagnet is indexed as 'L' ('R') .

Fig. 2 The magnetoresistances versus the bias voltage for non-interacting junction and the junctions with the space charge distribution. $\kappa_{0s}d = 300$ has been taken.

Fig. 3 The magnetoresistance versus λ_N/x_0 in V=0 for given semiconductor sizes x_0 . The curves corresponding to different l are plotted in each diagram.





